

```
chain nodes:
    1 2 3 4 7 8 9 10 11 12 13 14 15 16 17 18 27 28 29 30 31 32 33 34
    35 36 37

ring nodes:
    5 6 19 20 21 22 23 24 25 26

chain bonds:
    1-2 1-17 1-33 2-3 3-4 3-29 4-5 4-16 6-7 7-8 7-15 8-9 9-10 9-14 10-11 10-13
    11-12 11-18 14-20 26-27 26-28 29-30 29-31 29-32 33-34 34-35 34-36 34-37

ring bonds:
    5-6 5-24 6-23 19-20 19-22 20-21 21-22 23-25 23-26 24-25 25-26

exact/norm bonds:
    1-2 1-17 1-33 2-3 4-5 4-16 5-6 5-24 6-23 7-8 7-15 8-9 10-13 11-12 11-18
    19-20 19-22 20-21 21-22 23-25 23-26 24-25 25-26 33-34

exact bonds:
    3-4 3-29 6-7 9-10 9-14 10-11 14-20 26-27 26-28 29-30 29-31 29-32 34-35 34-36
    34-37
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Match level:
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS

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2 L5
L6
=> d l6 bib ab hitstr
     ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN
     2003:591204 CAPLUS
AN
     Preparation of peptides as NS3-serine protease inhibitors of hepatitis C
DN
ΤI
     Saksena, Anil K.; Girijavallabhn, Viyyoor M.; Lovey, Raymond G.; Jao,
     Edwin; Bennett, Frank; McCormick, Jinping L.; Wang, Haiyan; Pike, Russell
IN
     E.; Bogen, Stephane L.; Chan, Tin-yau; Liu, Yi-tsung; Zhu, Zhaoning;
     Njoroge, George F.; Arasappan, Ashok; Parekh, Tejal; Ganguly, Ashit K.;
     Chen, Kevin X.; Venkatraman, Srikanth; Vaccaro, Henry A.; Pinto, Patrick
     A.; Santhanam, Bama; Kemp, Scott Jeffrey; Levy, Odile Esther; Lim-Wilby,
     Marguerita; Tamura, Susan Y.; Wu, Wanli; Hendrata, Siska; Huang, Yuhua;
     Wong, Jesse K.; Nair, Latha G.
     Schering Corporation, USA; Corvas International, Inc.
 PΑ
     PCT Int. Appl., 633 pp.
 SO
     CODEN: PIXXD2
     Patent
 DT
     English
 LΑ
 FAN.CNT 1
                                           APPLICATION NO. DATE
                     KIND DATE
      PATENT NO.
                                           -----
      _____
                            _____
                                          WO 2003-US1430 20030116
                             20030731
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                      A2
      WO 2003062265
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              SL, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
          RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
              CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
              NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                       Α
                             20020118
 PRAI US 2002-52386
      MARPAT 139:149928
      The invention discloses novel peptides I [Y is alkyl, alkylaryl,
 OS
      heteroalkyl, heteroaryl, aryl- or alkylheteroaryl, cycloalkyl, alkyloxy,
 AΒ
      alkylaryloxy, aryloxy, heteroaryloxy, heterocycloalkyloxy, cycloalkyloxy,
      alkylamino, arylamino, alkylarylamino, arylamino, heteroarylamino,
      cycloalkylamino, or heterocycloalkylamino; R1 is acyl; Z is selected from
       O, N, CH or CR; R, R2-R4 are H, alkyl, alkenyl, cycloalkyl,
      heterocycloalkyl, alkoxy, aryloxy, alkylthio, arylthio, amino, amido,
       ester, carboxylic acid, carbamate, urea, ketone, aldehyde, cyano, nitro,
       halo, (cycloalkyl)alkyl, or (heterocycloalkyl)alkyl; W, Q, G, J, L, M
       independently may be present or absent; W is CO, CS, C(:N-CN), or SO2; Q
       is CH, N, P, alkylidene, O, NR, S, or SO2; A is O, CH, alkylidene, NR, S,
       SO2, or a bond; E is CH, N, alkylidene, or a double bond; G is alkylidene;
       J is alkylidene, SO2, NH, NR, or O; L is CH, CR, O, S, or NR; M is O, NR,
       S, SO2, or alkylidene (with provisos)] which have HCV protease inhibitory
       activity as well as methods for prepg. such compds. In another
       embodiment, the invention discloses pharmaceutical compns. comprising such
       compds. as well as methods of using them to treat disorders assocd. With
       the HCV protease. Thus, peptide \overline{\text{II}} was prepd. and showed \overline{\text{Ki}} = 1-100 nM
```

(category A) in the HCV continuous assay.

Absolute stereochemistry.

RN 395647-62-8 CAPLUS

CN 3-Azabicyclo[3.1.0] hexane-2-carboxamide, N-[3-amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[2-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-, (2S)- (9CI) (CA INDEX NAME)

RN 569677-40-3 CAPLUS
CN 3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-3-amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[(2S)-2-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-, (1R,2S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Me R
$$\frac{R}{R}$$
 $\frac{H}{N}$ $\frac{H}{N}$ $\frac{H}{N}$ $\frac{H}{N}$ $\frac{H}{N}$

RN 569677-41-4 CAPLUS
CN 3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1R)-3-amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[(2S)-2-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-, (1R,2S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Me R
$$\frac{R}{N}$$
 $\frac{R}{N}$ $\frac{H}{N}$ $\frac{H}{N}$ $\frac{R}{N}$ $\frac{H}{N}$ $\frac{H}{N}$

RN

3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[3-amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[(2S)-2-[[[(2-fluoro-1,1-dimethylethyl)amino]carbonyl]a CN mino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-, (1R,2S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

569677-85-6 CAPLUS

3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[3-amino-1-(cyclobutylmethyl)-RN 2,3-dioxopropyl]-3-[(2S)-3,3-dimethyl-1-oxo-2-[[[(2,2,2-trifluoro-1,1-CN

dimethylethyl)amino]carbonyl]amino]butyl]-6,6-dimethyl-, (1R,2S,5S)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.

RN 569678-27-9 CAPLUS
CN 3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[3-amino-1-[(1-fluorocyclobutyl)methyl]-2,3-dioxopropyl]-3-[(2S)-2-[[[(1,1-fluorocyclobutyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-, (1R,2S,5S)- (9CI) (CA INDEX NAME)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1937 TO DATE) 1 REFERENCES IN FILE CAPLUS (1937 TO DATE)

=> file caplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.42 54.49

FULL ESTIMATED COST

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FILE COVERS 1907 - 16 Sep 2003 VOL 139 ISS 12 FILE LAST UPDATED: 15 Sep 2003 (20030915/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s 12
               2 L2
L4
=> d l4 bib ab hitstr
     ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN
      2003:591204 CAPLUS
AN
      139:149928
DN
      Preparation of peptides as NS3-serine protease inhibitors of hepatitis C
ΤI
      Saksena, Anil K.; Girijavallabhn, Viyyoor M.; Lovey, Raymond G.; Jao,
IN
      Edwin; Bennett, Frank; McCormick, Jinping L.; Wang, Haiyan; Pike, Russell
      E.; Bogen, Stephane L.; Chan, Tin-yau; Liu, Yi-tsung; Zhu, Zhaoning;
      Njoroge, George F.; Arasappan, Ashok; Parekh, Tejal; Ganguly, Ashit K.;
      Chen, Kevin X.; Venkatraman, Srikanth; Vaccaro, Henry A.; Pinto, Patrick
      A.; Santhanam, Bama; Kemp, Scott Jeffrey; Levy, Odile Esther; Lim-Wilby,
      Marguerita; Tamura, Susan Y.; Wu, Wanli; Hendrata, Siska; Huang, Yuhua;
      Wong, Jesse K.; Nair, Latha G.
      Schering Corporation, USA; Corvas International, Inc.
PΑ
      PCT Int. Appl., 633 pp.
SO
      CODEN: PIXXD2
DT
      Patent
      English
LΑ
FAN.CNT 1
                                                  APPLICATION NO. DATE
                         KIND DATE
      PATENT NO.
                                                   _____
       _____
                                 _____
                                                  WO 2003-US1430 20030116
           W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SC, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZM, AT, BE, BG
                          A2 20030731
      WO 2003062265
 PΙ
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                ML, MR, NE, SN, TD, TG
                                  20020118
 PRAI US 2002-52386
                            Α
       MARPAT 139:149928
 OS
       The invention discloses novel peptides I [Y is alkyl, alkylaryl,
       heteroalkyl, heteroaryl, aryl- or alkylheteroaryl, cycloalkyl, alkyloxy,
       alkylaryloxy, aryloxy, heteroaryloxy, heterocycloalkyloxy, cycloalkyloxy,
       alkylamino, arylamino, alkylarylamino, arylamino, heteroarylamino,
       cycloalkylamino, or heterocycloalkylamino; R1 is acyl; Z is selected from
       O, N, CH or CR; R, R2-R4 are H, alkyl, alkenyl, cycloalkyl,
       heterocycloalkyl, alkoxy, aryloxy, alkylthio, arylthio, amino, amido,
       ester, carboxylic acid, carbamate, urea, ketone, aldehyde, cyano, nitro,
       halo, (cycloalkyl)alkyl, or (heterocycloalkyl)alkyl; W, Q, G, J, L, M
       independently may be present or absent; W is CO, CS, C(:N-CN), or SO2; Q
       is CH, N, P, alkylidene, O, NR, S, or SO2; A is O, CH, alkylidene, NR, S,
       SO2, or a bond; E is CH, N, alkylidene, or a double bond; G is alkylidene;
       J is alkylidene, SO2, NH, NR, or O; L is CH, CR, O, S, or NR; M is O, NR,
       S, SO2, or alkylidene (with provisos)] which have HCV protease inhibitory
       activity as well as methods for prepg. such compds. In another
        embodiment, the invention discloses pharmaceutical compns. comprising such
```

compds. as well as methods of using them to treat disorders assocd. with

the HCV protease. Thus, peptide II was prepd. and showed Ki = 1-100 nM (category A) in the HCV continuous assay.

394730-60-0P 395647-62-8P 569677-40-3P ΙT

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptides as NS3-serine protease inhibitors of hepatitis C virus)

RN

3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[3-amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[(2S)-2-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-CN dimethyl-1-oxobutyl]-6,6-dimethyl-, (1R,2S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Me
$$R$$
 R H_2N O

RN

3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[3-amino-1-(cyclobutylmethyl)-395647-62-8 CAPLUS 2,3-dioxopropyl]-3-[2-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-CN dimethyl-1-oxobutyl]-6,6-dimethyl-, (2S)- (9CI) (CA INDEX NAME)

RN 569677-40-3 CAPLUS

3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-3-amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[(2S)-2-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-(1R,2S,5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 569677-41-4 CAPLUS

CN 3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1R)-3-amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[(2S)-2-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-1, (1R,2S,5S)- (9CI) (CA INDEX NAME)